11. Electronic Structure in the d-p Model

AUTHOR(S):

神吉, 一樹

京都大学大学院 理学研究科 物理学第一専攻

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神 吉 一 樹

It has been established that the CuO_2 plane plays an essential role in high-T_c superconductivity. The on-site Coulomb repulsion U at Cu sites is large, and at zero-doping the system is an antiferromagnetic insulator. The nature of the states close to the Fermi level in doped systems has attracted intense interest. There are many experiments which indicate that the doped holes are more of O-$2p$ character than of Cu-$3d$ character. Some experiments are supposed to suggest that with hole-doping the Fermi level does not shift to the top of the valence band in the insulator phase , but that there develop new electronic states at the Fermi level. These states are sometimes called 'impurity states' or 'mid-gap states', although the nature of these states is not known clearly.

There have been many theoretical studies to know the nature of quasiparticles or electronic states at the Fermi level , and there are some theoretical attempts to demonstrate the appearance of the 'mid-gap states'. In these works they considered the infinite U limit treating the transfer terms as perturbation, in other words these are approaches from the insulator phase or the atomic limit.

Although U is large in this system , it is a natural approach to introduce the electron-interaction into a non-interacting system, as long as the system remains a Fermi liquid. Moreover it is expected that a Fermion system develops continuously from a non-interacting system through introduction of interactions. In other words, physical quantities for a Fermi liquid should be analytic functions of interaction strength. Therefore in the present work the d-p model is studied by the perturbation method with respect to U. In this model Cu $d_{x^2-y^2}$ orbitals hybridize with O $p_{x,y}$ orbitals with the transfer integral t. For simplicity p_x-p_y direct transfer, on-site Coulomb repulsion at O-sites, and inter-atomic Coulomb energy are neglected. In order to take account of the interaction the d-electron selfenergy $\Sigma_k(\omega)$ should be calculated. In this work an attempt has been made to calculate the second order term of the selfenergy. In such calculation it is necessary to execute a $2d$-fold momentum integration on a integrand which has a pole structure , where d is the dimension of the system. As a result it is difficult

to study the realistic two-dimensional model, therefore calculation has been done on a one-dimensional model. It is expected that the present calculation would reveal the essential electronic structure, except for some structures due to one-dimensionality. In the absence of interaction there are two bands, which are constructed by the d-p transfer.

With the p-level and d-level given by the Hartree-Fock solution fixed at $-1.0t$ and $-2.0t$, respectively , density of states has been calculated for various values of U. In the d-electron density of states there appear some states which tend to develop into the lower and upper Hubbard bands. There always exist some states around the Fermi level. With increasing U, increases the ratio of the d-electron density of states to the p-electron part at the Fermi level. This is because the d-level shifts nearer to the Fermi level due to the positive selfenergy at the Fermi level.

It has been found that there is no structure which corresponds to the 'mid-gap states'. The imaginary part of the selfenergy vanishes at the Fermi level , and rises linearly in ω. The real part of the selfenergy has no particular structure around the Fermi level, except the anomaly due to one-dimensionality. Therefore no peak structure corresponding to the 'mid-gap states' is expected in the present second order U-perturbation treatment. It seems that there is no need to consider the states at the Fermi level to be anything particular like 'impurity states', as long as we are studying the normal state properties in the approach from the metallic side.

The mass enhancement factor $\left(1-\left.\frac{\partial \Sigma_k(\omega)}{\partial \omega}\right|_{\omega\approx 0}\right)$ is estimated to be of the order of unity. In comparison to similar calculations on the periodic Anderson model, which is studied as a model of heavy electron systems, it is expected that mass enhancement is not so large in the present system.

12. レーザースノーの成長過程における諸形態

佐 飛 裕 一

水素ガス中のアルカリ金属原子にレーザー光を照射すると、光線中でアルカリ水素分子が大量に生成し、1μm大の結晶微粒子に凝縮し落下する。これはレ